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ON CHANGING INTERCYCLE CORRELATION IN MONTE CARLO K-EIGENVALUE CALCULATION

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ABSTRACT

The present paper investigates the possibility of reducing the intercycle source correlation in Monte Carlo (MC) $k-$eigenvalue calculation and thereby raising the reliability of its error estimation. To this end, a large medium with a localized highly multiplying region has been chosen as a test problem because the statistical error estimation by sample variance tends to be significantly underestimated, and such a medium is encountered in the simulation of a whole reactor core with a sharp power peak. A key principle is to confine MC particles in a small region and make the computational domain virtually smaller than its actual physical size. The exponential transform for path-stretching has been employed to implement that principle. To demonstrate the reduction of the intercycle source correlation, numerical results are shown for real and apparent variance.

I. INTRODUCTION

In MC $k-$eigenvalue calculation, the statistical error is estimated through sample variance by many practitioners. As shown in standard introductory statistics textbooks (Larsen, 1986), sample variance is unbiased when there exists no correlation among samples. However, the recursive nature of iterative source cycles makes samples of $k-$eigenvalues correlated and the estimated standard deviation is therefore biased. A straightforward method to cope with the bias problem is to calculate the sample variance of batches of $k-$samples since the virtual lag between the adjacent batches increases. Gelbard and Prael investigated the performance of the batch method (Gelbard, 1990). There are some relations among real and apparent variance and lag-covariances, where “real” refers to the variance of sample mean and the lag-covariance of samples, and “apparent” to the expected value of the sample variance and lag-covariances. Based on these relations, Ueki et al. proposed an iterative method to estimate real variance (Ueki, 1997). Demaret et al. and Jacquet et al. analyzed both these methods and showed that the batch method might become unstable and be still biased for a problem where the correlation among $k-$samples is large, and the iterative method is unbiased but generally unstable(Demaret, 1999, Jaquet, 2000). They proposed a fitting method of estimating lag-covariances based on time series methodologies and showed that it stably performs. At the current stage, it is fair to say that the fitting method is robust due to the stability.

The present paper investigates the possibility of reducing the intercycle correlation of sources and thereby the correlation among $k-$samples to improve the reliability of MC $k-$error estimation. No attempt is made at modifying the procedure of source iteration and normalization. It would be best to devise a method to eliminate the error estimation bias. The present paper is however motivated by the observation that methods for improved error estimation including the foregoing work often perform satisfactorily when the correlation among samples is sufficiently small. A large medium with a localized highly multiplying region has been chosen as a test problem because the statistical error could be significantly underestimated and such a medium would be encountered in the simulation of a whole reactor core with a sharp power peak. For example, the boiling water reactor core at a cold or hot standby becomes such a medium when a control rod has accidentally dropped. Qualitatively, a certain fraction of the MC particles in a sharp distribution peak tend to escape from that peak and spread over the surrounding region. Since the movement of one MC particle can cover only a small area in one cycle, the statistical fluctuation of the source caused by those spreading particles at one cycle tends to be transfered to the next cycle and the intercycle source correlation consequently becomes positively large. To suppress such a phenomenon, we attempt at the fair biasing of MC transport processes to confine MC particles in a highly multiplying region and make the computational domain virtually smaller than its actual physical size. To this end, the exponential transform for path stretching (Kahn, 1949, Lux, 1991) has been employed contrary to the traditional usage in deep penetration problems. As an indirect demonstration of the reduction of the intercycle source correlation, numerical results are shown for real variance, which is the variance of sample mean, and apparent variance, which is the expected value of sample variance.

II. STATISTICAL TREATMENTS

A quantity of interest is the variance of the eigenvalue estimate k:

$$k = \frac{1}{N}\sum_{j=1}^{N} k_j. \tag{1}$$

where k_j is the eigenvalue estimate at the j-th stationary cycle and N is the number of cycles after the source reached stationarity. A standard estimator of the variance of k is sample variance:

$$\sigma_S^2 = \frac{1}{N(N-1)}\sum_{i=1}^{N}(k_i - k)^2. \tag{2}$$

The expected value of σ_S^2, which is called apparent variance and denoted by σ_A^2, is calculated by

$$\sigma_A^2 \approx \frac{1}{M}\sum_{i=1}^{M}\frac{1}{N(N-1)}\sum_{j=1}^{N}\left(k_j^i - \frac{1}{N}\sum_{m=1}^{N} k_m^i \right)^2 \tag{3}$$

where M is the number of independently replicated Monte Carlo runs, N is the number of stationary cycles per run and k_j^i is the eigenvalue estimate at the j-th stationary cycle of the i-th run. In general, the apparent variance is not equal to real variance that is denoted by σ_R^2 and defined by

$$\sigma_R^2 = E[k^2] - E[k]^2, \tag{4}$$

because of the following relation (Ueki, 1997):

$$\sigma_A^2 - \sigma_R^2 = -\frac{2}{N(N-1)} \sum_{i=1}^{N} (N-i) C_R[i], \tag{5}$$

where $C_R[i]$ is real lag-i covariance:

$$C_R[i] = E[(k_m - E[k])(k_{m+i} - E[k])],\ m = 1, \ldots, N-i. \tag{6}$$

Note that the stationarity dictates that $E[k] = E[k_m] = E[k_{m+i}]$ and $C_R[i]$ is independent of m. The real variance is calculated by

$$\sigma_R^2 \approx \frac{1}{M-1} \sum_{i=1}^{M} \Big(\frac{1}{N} \sum_{j=1}^{N} k_j^i - \frac{1}{M} \sum_{i=1}^{M} \frac{1}{N} \sum_{j=1}^{N} k_j^i \Big)^2. \tag{7}$$

Eqs. (3) and (7) are used in the later section for numerical results.

III. EXPONENTIAL TRANSFORM OF A $K-$EIGENVALUE PROBLEM

We describe the exponential transform for path stretching (Kahn, 1949, Lux, 1991) for the $k-$eigenvalue problem of a two-dimensional medium with no energy dependence and isotropic scattering. The transport equation for angular flux ψ is

$$\begin{aligned}
&\mu_x \frac{\partial \psi(x,y,\mu_z,\phi)}{\partial x} + \mu_y \frac{\partial \psi(x,y,\mu_z,\phi)}{\partial y} + \sigma_t \psi(x,y,\mu_z,\phi) \\
&\quad = \frac{\sigma_{s0}}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} \psi(x,y,\mu_z',\phi')\, d\phi'\, d\mu_z' + \frac{1}{k} \frac{\nu\sigma_f}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} \psi(x,y,\mu_z',\phi')\, d\phi'\, d\mu_z', \\
&\qquad -d < x < d\ ,\ -e < y < e\ ,\ -1 \le \mu_z \le 1\ ,\ 0 \le \phi \le 2\pi\ ,
\end{aligned} \tag{8}$$

$$\psi(-d,y,\mu_z,\phi) = 0\ ,\ 0 \le \phi < \frac{\pi}{2}\ ,\ \frac{3\pi}{2} < \phi \le 2\pi\ ,\ -e < y < e\ , \tag{9}$$

$$\psi(x,-e,\mu_z,\phi) = 0\ ,\ 0 < \phi < \pi\ ,\ -d < x < d\ , \tag{10}$$

$$\psi(d,y,\mu_z,\phi) = 0\ ,\ \frac{\pi}{2} < \phi < \frac{3\pi}{2}\ ,\ -e < y < e\ , \tag{11}$$

$$\psi(x,e,\mu_z,\phi) = 0\ ,\ \pi < \phi < 2\pi\ ,\ -d < x < d\ , \tag{12}$$

where σ's and ν are standard notations, and the variables for solid angles are defined as:

μ_z = 'cosine of the polar angle about z axis',

$\phi =$ 'azimuthal angle around z axis',

$\mu_x = \sqrt{1-\mu_z^2}\cos\phi$

$\mu_y = \sqrt{1-\mu_z^2}\sin\phi$.

We consider a different transport problem by the following exponential transformation:

$$\Psi(x,y,\mu_z,\phi) = \begin{cases} \psi(x,y,\mu_z,\phi)e^{-\lambda_x\sigma_t(x-a)-\lambda_y\sigma_t(y-b)}\,, & a<x<d,\ b<y<e, \\ \psi(x,y,\mu_z,\phi)e^{-\lambda_y\sigma_t(y-b)}\,, & -a<x<a,\ b<y<e, \\ \psi(x,y,\mu_z,\phi)e^{\lambda_x\sigma_t(x+a)-\lambda_y\sigma_t(y-b)}\,, & -d<x<-a,\ b<y<e, \\ \psi(x,y,\mu_z,\phi)e^{\lambda_x\sigma_t(x+a)}\,, & -d<x<-a,\ -b<y<b, \\ \psi(x,y,\mu_z,\phi)e^{\lambda_x\sigma_t(x+a)+\lambda_y\sigma_t(y+b)}\,, & -d<x<-a,\ -e<y<-b, \\ \psi(x,y,\mu_z,\phi)e^{\lambda_y\sigma_t(y+b)}\,, & -a<x<a,\ -e<y<-b, \\ \psi(x,y,\mu_z,\phi)e^{-\lambda_x\sigma_t(x-a)+\lambda_y\sigma_t(y+b)}\,, & a<x<d,\ -e<y<-b, \\ \psi(x,y,\mu_z,\phi)e^{-\lambda_x\sigma_t(x-a)}\,, & a<x<d,\ -b<y<b, \\ \psi(x,y,\mu_z,\phi)\,, & -a<x<a,\ -b<y<b, \end{cases} \tag{13}$$

where $0<a<d$ and $0<b<e$. The substitution of (13) into Eqs. (8)-(12) yields

$$\begin{aligned} &\mu_x\frac{\partial\Psi(x,y,\mu_z,\phi)}{\partial x}+\mu_y\frac{\partial\Psi(x,y,\mu_z,\phi)}{\partial y}+\sigma_t(1+\vec{\Lambda}\cdot\vec{\Omega})\Psi(x,y,\mu_z,\phi) \\ &\quad=\frac{1}{4\pi}\int_{-1}^{1}\int_0^{2\pi}\sigma_t(1+\vec{\Lambda}\cdot\vec{\Omega}')\Psi(x,y,\mu_z',\phi')\frac{\sigma_{s0}}{\sigma_t(1+\vec{\Lambda}\cdot\vec{\Omega}')}\,d\phi'\,d\mu_z' \\ &\qquad+\frac{1}{k}\frac{1}{4\pi}\int_{-1}^{1}\int_0^{2\pi}\sigma_t(1+\vec{\Lambda}\cdot\vec{\Omega}')\Psi(x,y,\mu_z',\phi')\frac{\nu\sigma_f}{\sigma_t(1+\vec{\Lambda}\cdot\vec{\Omega}')}\,d\phi'\,d\mu_z'\,, \\ &\qquad -d<x<d\,,\ -e<y<e\,,\ -1\le\mu_z\le 1\,,\ 0\le\phi\le 2\pi\,, \end{aligned} \tag{14}$$

$$\Psi(-d,y,\mu_z,\phi)=0\,,\ 0\le\phi<\frac{\pi}{2}\,,\ \frac{3\pi}{2}<\phi\le 2\pi\,,\ -e<y<e\,, \tag{15}$$

$$\Psi(x,-e,\mu_z,\phi)=0\,,\ 0<\phi<\pi\,,\ -d<x<d\,, \tag{16}$$

$$\Psi(d,y,\mu_z,\phi)=0\,,\ \frac{\pi}{2}<\phi<\frac{3\pi}{2}\,,\ -e<y<e\,, \tag{17}$$

$$\Psi(x,e,\mu_z,\phi)=0\,,\ \pi<\phi<2\pi\,,\ -d<x<d\,, \tag{18}$$

where $\vec{\Omega}$ and $\vec{\Lambda}$ are defined as:

$$\vec{\Omega}=(\mu_x,\mu_y,\mu_z),$$

and

$$\vec{\Lambda} = \begin{cases} (\lambda_x, \lambda_y, 0) & \text{for } a < x < d \text{ and } b < y < e\,, \\ (0, \lambda_y, 0) & \text{for } -a < x < a \text{ and } b < y < e\,, \\ (-\lambda_x, \lambda_y, 0) & \text{for } -d < x < -a \text{ and } b < y < e\,, \\ (-\lambda_x, 0, 0) & \text{for } -d < x < -a \text{ and } -b < y < b\,, \\ (-\lambda_x, -\lambda_y, 0) & \text{for } -d < x < -a \text{ and } -e < y < -b\,, \\ (0, -\lambda_y, 0) & \text{for } -a < x < a \text{ and } -e < y < -b\,, \\ (\lambda_x, -\lambda_y, 0) & \text{for } a < x < d \text{ and } -e < y < -b\,, \\ (\lambda_x, 0, 0) & \text{for } a < x < d \text{ and } -b < y < b\,, \\ (0, 0, 0) & \text{for } -a < x < a \text{ and } -b < y < b\,. \end{cases}$$

The transformed transport processes in Eq. (14) are interpreted as

$\sigma_t(1 + \vec{\Lambda} \cdot \vec{\Omega})$ = total macroscopic cross section for particles moving in direction $\vec{\Omega}$,

$\sigma_{s0}/[\sigma_t(1 + \vec{\Lambda} \cdot \vec{\Omega}')]$ = mean number of particles emerging from scattering per collision event of particles moving in direction $\vec{\Omega}'$,

$\nu\sigma_f/[\sigma_t(1+\vec{\Lambda}\cdot\vec{\Omega}')]$ = mean number of particles emerging from fission per collision event of particles moving in direction $\vec{\Omega}'$,

and the direction of movement after scattering or fission is isotropic. Thus, in the transport processes dictated by Eq. (14), particles are nearly confined in and near the central region $-a < x < a$ and $-b < y < b$ when both λ_x and λ_y are positive. In the next section, the central region is made highly multiplying to yield the sharp distribution peak of physical particles. The exponential transform makes the distribution peak of the particles dictated by Eqs. (14)-(18) sharper than that of the particles dictated by Eqs. (8)-(12).

IV. NUMERICAL RESULTS

The present section shows two sets of numerical results about the real and apparent standard deviations, σ_A and σ_R, for various values of the exponential transform parameters. Its purpose is to indirectly demonstrate the reduction of the intercycle correlation of sources from which particle's initial variables are sampled to compute k_j's or k_j^i's. Implicit capture with Russian roulette (RR) was employed. k_j^i's were estimated by independently replicated 500 runs. In a single run, 300 cycles were recursively iterated of which the first 100 cycles were disposed to secure stationarity. Thus, $N = 200$ and $M = 500$. The number of particle's histories per cycle is 2000.

The first problem is shown in Figure 1. The central highly multiplying region is taken to be non-transform region ($-a < x < a$, $-b < y < b$). The apparent and real standard deviations are shown in Figure 2. It is observed that the error estimation bias, $|\sigma_A - \sigma_R|$, is significantly reduced together with the decrease of σ_R when the transform parameter is chosen optimally. It is also observed that both $|\sigma_A - \sigma_R|$ and

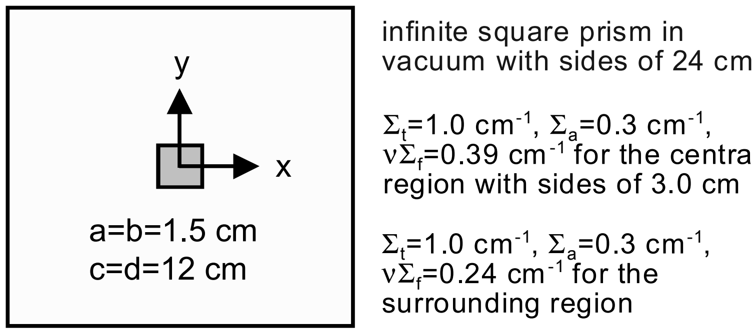

Figure 1: Two dimensional heterogeneous problem

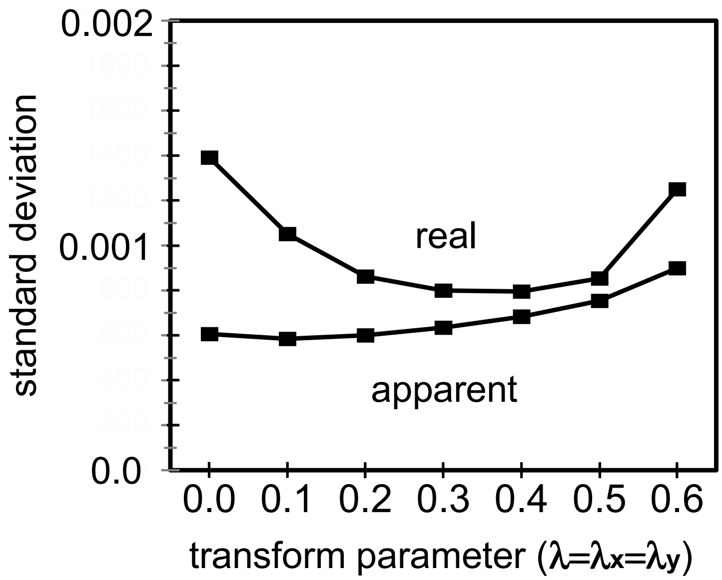

Figure 2: Real and apparent standard deviation for two dimensional heterogeneous problem in Figure 1

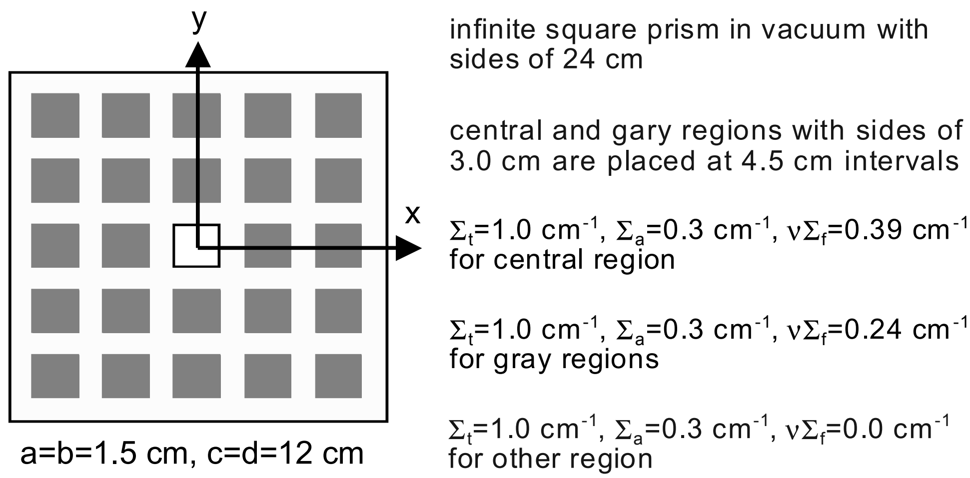

Figure 3: Two dimensional heterogeneous problem with non-fissionable region

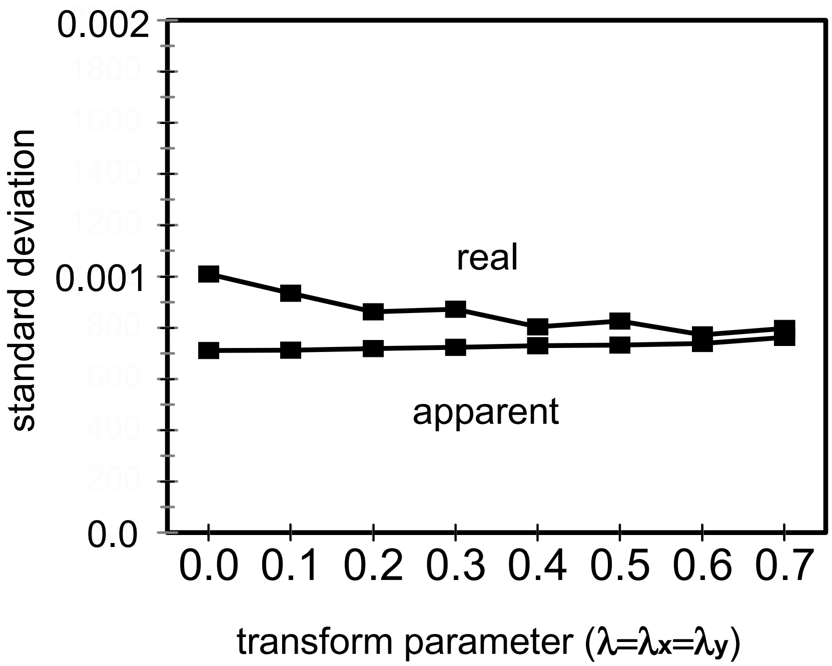

Figure 4: Real and apparent standard deviation of two dimensional heterogeneous problem with non-fissionable region in Figure 3

σ_R start to increase beyond that optimal parameter value. The increase of σ_R could be explained by the increase of the fluctuation of statistical weights. However, the present author has not found a reasonable explanation for the increase of $|\sigma_A - \sigma_R|$ although it could be qualitatively argued that larger values of λ_x and λ_y tend to keep the particle's overpopulation at the central region caused by the statistical fluctuation of the source. The second problem is two dimensional periodical array shown in Figure 3. The central highly multiplying region is again taken to be non-transform region. Numerical results are shown in Figure 4. As in the first problem, the error estimation bias is reduced, but the optimal value of the transform parameter appears to be larger than that of the first problem. Both λ_x and λ_y are taken to be smaller than 0.7 because $|\vec{\Lambda}| = \sqrt{\lambda_x^2 + \lambda_y^2}$ and $\lambda_x = \lambda_y$ in $a < x < d$ and $b < y < e$, $-d < x < -a$ and $b < y < e$, $-d < x < -a$ and $-e < y < -b$, and $a < x < d$ and $-e < y < -b$. The increase of $|\sigma_A - \sigma_R|$ was not observed.

In the following, we discuss issues related to the numerical results presented:

1. Real standard deviation decreased in both numerical results. Previous work for the variance reduction in MC eigenvalue calculation did not clearly differentiate real and apparent variance (Whitesides, 1968). The present work makes caution on that. The strategy of variance reduction research should be $\sigma_A \downarrow 0$ and $\sigma_A/\sigma_R \rightarrow 1$. If σ_A/σ_R is made sufficiently close to unity, the batch method will nearly eliminate the $k-$error estimation bias.

2. We did not investigate the so-called loosely coupled system like a collection of fissionable components separated by air. Angular biasing of the direction of movement at post-collision would be useful to such a system.

3. The parameter settings of RR affect the relative bias in error estimation, $(\sigma_A - \sigma_R)/\sigma_R$. In this section, the threshold weight to perform RR is 0.3, the weight after RR was performed is 0.3, and initial weight is unity.

4. Performance comparison was not made with superhistory powering (Brissenden, 1986). It is a method for source iteration and normalization, wherein the biasing of particle transport processes like the exponential transform can be implemented to reduce the intercycle correlation and thereby shorten the length of a sequence of unnormalized cycles.

V. SUMMARY

The present paper has shown the possibility of changing the intercycle source correlation in MC $k-$eigenvalue calculation with no change in source normalization procedures.

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